Yucca Mountain Site Characterization Project (YMP)

Site Characterization and Modeling

3-D Mineralogical Model of Yucca Mountain

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To prepare for the 2001 license application for the potential repository at Yucca Mountain, an integrated site model of the geology and hydrology site has been developed through collaborations at the national level. It will merge the detailed stratigraphy, rock properties, and mineralogical data previously collected into a 3-D model of the Yucca Mountain area. This integrated site model will then be used in process models of repository performance (e.g., hydrologic flow, and radionuclide transport), which will then be incorporated into the Total System Performance Assessment (TSPA) model of the repository block and vicinity. The results of the TSPA will determine if Yucca Mountain is a suitable site for the repository.

Our role in building the integrated site model has been to generate a 3-D mineralogic model based on a comprehensive analysis of mineralogical data from borehole samples, using numerical methods derived from the petroleum industry. We obtained this information over the last 20 years by examining Yucca Mountain data from 24 boreholes, surface geologic maps, and tunnel excavations. We are generating a new version of the mineralogical model that will integrate geophysical borehole measurements with the x-ray diffraction data. This latest version will also provide a more internally consistent picture of the relationship between zeolite abundance and permeability, a critical issue for researchers modeling radionuclide transport, since the zeolite's high sorptive capacity will clearly influence the transport of radionuclides away from the repository.

Advanced Meshes for Geologic Computation

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Mesh generation is a critical aspect of many of the computational modeling projects for the YMP and for other EES programs (Environmental Restoration and Hard and Deeply Buried Targets). We are collaborating with T and X Divisions to develop and apply advanced tools to unstructured finite-element and finite-volume mesh generation. Whereas the algorithms and methods in these tools are quite general, their development has been driven by applications in shock physics, semiconductor device modeling, grain growth, and porous flow.

Los Alamos Grid Toolbox (LaGriT) is a library of user-callable tools that provide mesh generation, mesh optimization, and dynamic mesh maintenance in three dimensions for a variety of applications. Geometric regions within arbitrarily complicated geometries are defined as combinations of bounding surfaces, whereas the surfaces are described analytically or as piecewise linear tessellations. A variety of techniques for distributing points within these geometric regions are provided. Mesh generation uses an algorithm that respects material interfaces and ensures that there are no negative coupling coefficients in the associated Voronoi control volumes. The data structures created to implement this algorithm are compact and powerful, and they are expandable to include hybrid meshes, as well as tetrahedral meshes.

Mesh refinement and smoothing are available to modify the mesh to provide more resolution in areas of interest. Mesh refinement adds nodes to the mesh based on geometric criteria such as edge length or based on field-variable values or gradients. Mesh elements may become distorted as mesh nodes move during a time criteria such as change in field. Mesh smoothing moves nodes to adapt the mesh to field-variable measures, and, at the same time, maintains quality element-dependent simulation or adds nodes, as a result of refinement operations. Mesh reconnection via a series of edge flips will maintain the non-negative coupling coefficient criterion of the mesh while eliminating highly distorted elements.

Unsaturated-Zone Transport Test (UZTT) at Busted Butte

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Busted Butte, Nevada, is the site of an ongoing unsaturated-zone tracer test designed to address solute and colloid movement through tuff horizons that underlie the potential high-level nuclear waste repository at Yucca Mountain. Busted Butte was selected as the location for this test because at Busted Butte, the geologic layers that underlie the proposed repository have been faulted up to the surface. Thus, Busted Butte is an analog site for both the vitric Calico Hills Formation and the Topopah Spring Tuff units as they exist beneath the potential repository horizon west of the Ghost Dance fault. The principal objectives of this test are to evaluate (1) the 3-D site-scale flow-and-transport process model used in the Yucca Mountain Total System Performance Assessment; (2) the effect of heterogeneities on flow and transport in unsaturated and partially saturated conditions in the Calico Hills formation; (3) the effect of scaling from lab scale to field scale and site scale; (4) the validation of laboratory sorption experiments using field tests in unsaturated Calico Hills rocks; and (5) the migration behavior of colloids in fractured and unfractured Calico Hills rocks.

For this report we will focus on Phase 2 of the UZTT. This phase is an integrated field, laboratory, and modeling effort to quantify the effects of hydrogeologic conditions operative at the potential Yucca Mountain repository site. We inject aqueous tracers into the rock through horizontal boreholes, measure tracer migration at collection boreholes or by mine back, and then we will compare those measurements with our modeling predictions. We are conducting in situ experiments on a 10 x 10 x 7-m block, which consists of layers of the Topopah Springs and Calico Hills formations, with two embedded faults. Tracer solution is continuously injected from eight parallel boreholes in two horizontal planes. Injection rates range from 1 to 50 mL/h. The injection mixtures consist of both nonreactive and reactive tracers, including halides, metals, synthetic colloids, and organic dyes. Each mixture also includes one of five different fluorinated benzoic acids, which enables tracking the tracer from specific injection boreholes. Fifteen collection boreholes are emplaced perpendicular to injection holes, and they are both horizontal and inclined. Pore-water samples are collected regularly from these holes, using sorbing paper-collection pads. Injection-to-collection travel distances range from 15 to 700 cm.

Our computational model uses an unstructured grid that accurately represents the size and location of each borehole and injection point, the unit boundaries, and the faults. Using FEHM, we are running simulations using parameters most representative of the UZTT. Hydrogeologic parameters are taken from measurements at Busted Butte, as available, and from the YMP database otherwise. Our results demonstrate excellent qualitative agreement and strong quantitative agreement between model and analysis. The modeling is able to capture the breakthrough, overall shape of the tracer fronts in time, and the extent of mixing of tagged tracers.

Understanding the role of scaling and travel distance is one UZTT objective. To assess the impact of travel distance, we placed collection holes at various distances from the injection holes. By varying the travel distance, we have provided a range of scales for studying transport, from tens of centimeters to meters. Breakthrough times at the various distances scale approximately linearly with travel distance. Fifty percent breakthrough of bromide in borehole 16 occurs at just under 125 days, whereas at borehole 15, almost twice as far from the injection holes, breakthrough occurs at approximately 250 days.

Qualitative agreement is very good between our model and the data, with the model representing borehole effects and layering. The actual injection rate appears to be 10 to 20% lower than the planned rate. The quantitative quality of fit is reduced for the actual injection rate versus the designed rate simulations. The fact that the quality of fit uniformly decreases with change in injection rate suggests the possibility that scaling effects are significant, and that the

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laboratory-measured hydrogeologic parameters do not accurately reflect the field behavior. For example, if reported laboratory conductivities are lower than the effective field conductivities, the model would underpredict breakthrough. Underprediction of conductivity in the laboratory is likely because these tests are run on samples that are recoverable. More permeable samples tend to disintegrate in the field, so they are not tested in the laboratory. These issues are currently being tested.

Verifying FEHM

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FEHM (finite-element heat and mass-transfer code) was originally developed at Los Alamos in the early 1980s to simulate geothermal and hot dry rock reservoirs. This code has been used to model other contaminant transport problems at over 100 sites around the world.

We work with the Los Alamos YMP Quality Assurance section to verify each version of FEHM, which has been used extensively since 1990 by the YMP. The code is used to model nonisothermal, multiphase, multicomponent flow and solute transport in porous media. It is applicable to natural-state studies of geothermal systems, groundwater flow, and solute transport.

The FEHM baseline update for the YMP was verified in April 1999. The update involved converting the program to Fortran 90 and adding additional functionality. The verification process, mandated by DOE quality assurance requirements, consists of rigorous testing of the model against known analytical solutions to the same problem. For more complex test cases for which no analytical solutions exist, we benchmark the code against numerical modeling results. We test each major FEHM submodel (heat transfer, isothermal fluid flow, coupled heat and mass transfer, and solute transport) using analytic solutions or benchmarking. To ensure that accuracy and quality are maintained as part of the code development process, we have developed a series of tests that we regularly run on the code. Over the past year, we added additional functionality to the code and expanded the number of verification test cases. A baseline update of FEHM was completed in December 2000.

Saturated-Zone Flow and Transport

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The saturated zone beneath Yucca Mountain is an important natural barrier to migration of radionuclides away from the proposed repository. To understand the basic flow mechanisms that govern flow and transport in the groundwater system at Yucca Mountain, we need to develop a conceptual model of the flow system. In particular, the model must include fracture flow in a geologic framework dominated by large faults. This project involves development of such a model, generation of an associated computational grid, calibration of the model to known water levels and hydraulic heads, and computer simulations of radionuclide transport. The objective is to provide a defensible site-scale flow and transport model for the saturated zone that can be part of the Total System Performance Assessment of the proposed repository at Yucca Mountain.

Our conceptual model for transport includes fracture pathways with substantial radionuclide diffusion from the fractures into the rock matrix. Our grid-generation process uses a sequence of grids to capture details of a hydrologic framework model developed by collaborators at the USGS. One goal of this sequence approach was to quantify numerical errors. The calibration process combines FEHM, with a commercial parameter estimation code (PEST) to determine water-flow permeability values for the hydrologic units that best fit the observed data. We use the calibrated flow field to simulate potential radionuclide flow paths. Our simulated paths agree with those determined using known geochemical data from Yucca Mountain and the surrounding region.

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Recent work on the model includes testing a fine grid imbedded in the previous model that doubles (and eventually quadruples) the resolution around Yucca Mountain. We will use this new grid to simulate recent multiwell tracer tests and to design new multiwell experiments. In addition, we plan to carry out a sensitivity study concerning the pre- and post-development boundary conditions of the potential repository.

Mineralogy Studies for the Single-Heater Test

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The thermal test program at Yucca Mountain began by studying the coupled thermal, hydrologic, and chemical processes that occurred during a prototype heating test (Single-Heater Test), simulating the effects of radioactive waste emplacement in the underground repository. Evidence of mineralogic change during the nine-month heating period was an important aspect of the test. Conceptual and numerical models predicted that water vapor would be driven away from the hottest region surrounding the heater, condense beyond the boiling front, and flow downward back to the dry-out region. We asked two questions. What happened to the devitrified, welded tuff as it was heated and interacted with moving water? Did mineral dissolution and deposition occur within the fracture system that conducted the water?

Because the Single-Heater Test was a prototype experiment, the mineralogic studies focused on identifying minerals deposited during the test, rather than conducting a complete analysis of the test effects. Overcores of the original pretest boreholes were examined by scanning-electron microscopy for evidence of new mineral deposition, and mineral identifications were confirmed by quantitative x-ray diffraction analysis. The major mineral products of the test were calcite, gypsum, and amorphous silica. Prototype characterization efforts also included a detailed inventory of stellerite (a zeolite) present on fracture surfaces in pretest drill core, providing input on this parameter to the numerical simulations of the heater test.

Our results confirmed that mineral deposition occurred in fractures during the test, a process that could significantly alter the permeability of the rock mass over time. Our results also suggested that alteration of the rock matrix was very minimal. The experience gained from this test has helped us develop expertise in the specialized area of field-test mineralogic characterization, particularly as it applies to geochemical modeling.

Mineralogy-Petrology Studies for the Drift-Scale Test and the Unsaturated-Zone Transport Test (UZTT) at Busted Butte

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The YMP is conducting several long-term field tests to evaluate the possible effects of nuclear waste emplacement in the potential Yucca Mountain geologic repository. We are participating in two of these field tests, the underground Drift-Scale Test (DST) and the Unsaturated-Zone Transport Test at Busted Butte. The DST is designed to study the coupled thermal-mechanical-hydrologic-chemical responses of a rock mass at up to 200ºC. We are investigating the mineralogical and chemical effects of natural pore fluids migrating through the rock in response to heating, and we are providing input to those conducting numerical simulations of coupled processes. We have mapped stellerite and other natural mineral distributions in fractures in the Single-Heater and DST blocks and have identified Single-Heater Test mineral products, as described above. Based on our results, we provide potential targets for in-progress mineralogic sampling to the field testers. The recovered sidewall samples do contain new mineral deposits that are being studied.

For the UZTT at Busted Butte, we evaluated the mineralogy and lithology of Busted Butte before the test facility was sited, and we have documented the mineralogy of rocks in the test blocks to allow comparisons with Yucca

Mineralogy-Petrology Studies for the Drift-Scale Test and the UZTT

Mountain mineralogy and to help model the sorption behavior of nonconservative tracers. We have also flagged stratigraphic units in test blocks, performed auger sampling in floor of test facility, x-ray diffraction analysis of selected samples, and mapping of mineback faces. Our mapping of faults within the test blocks, based on drill-core study and bore-hole-televiewer analysis, will be incorporated into numerical simulations of the tracer tests.

Paiute Ridge Natural Analogue Study

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In a fortuitous set of events, nature may have provided a natural analogue for studying the effects the potential Yucca Mountain repository may have on the surrounding tuffaceous host rock in which the repository may be placed. We are studying dike and sill complexes that intruded tuffaceous host rocks above the water table at the Nevada Test Site as possible analogues for thermal-hydrologic-chemical coupled processes expected for the Yucca Mountain repository. Heat produced by the repository is expected to result in the formation of heat pipes with counterflow of liquid water and water vapor both above and below the repository horizon. Alteration of the host rock can be expected as a result of the boiling conditions. However, the extent of alteration is unknown, and it is hoped that natural analogues can shed light on the degree of alteration to expect. Papoose Lake sill, on the northern edge of Paiute Ridge intrusive complex, is being characterized by mapping rock alteration and stratigraphy, and determining the pre-intrusive alteration state of the host rocks. Field work will be combined with modeling studies of rock alteration resulting from two-phase flow and transport processes.

Transport of Colloids in the Unsaturated Zone

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The thick unsaturated zone between the water table and the potential repository at Yucca Mountain serves as a natural barrier for the transport of radionuclides to the environment. However, this barrier could be circumvented if actinides were to sorb onto and be carried away by colloids present in water percolating through the system. We are investigating the possibility of such colloid-facilitated transport through the unsaturated zone at Yucca Mountain. Waste-form colloids, clay colloids formed from the weathering of waste glass, have been identified as having the largest risk for colloid-facilitated transport in the unsaturated zone. As a result, ours was the only colloid-transport scenario investigated using a process-level model (a discrete fracture model) to understand the important mechanisms and to develop an abstracted particle-tracking model for the Total System Performance Assessment (TSPA) being conducted at the national level.

There are very few site-specific data on colloid transport through volcanic tuffs at Yucca Mountain. Therefore, to account for physical removal of colloids, we used moisture retention data collected on core samples to derive pore-size distributions for the different stratigraphic units and, then, based on the colloid size of interest, determined a probability for colloids entering a particular unit in the saturated zone. This relationship was used in our process-level model as a size-exclusion factor for determining the distribution of colloids between the fracture and rock-matrix units. In the particle-tracking model for TSPA, we incorporated an additional relationship based on pore-size distributions that allowed us to examine colloid filtration at matrix-matrix interfaces. We also used filtration theory to evaluate colloid removal in the fracture and rock-matrix units. Because we did not account for the influence of solution chemistry, volumetric

Transport of Colloids in the Unsaturated Zone

water content, fracture roughness, and chemical properties of the colloids—all factors that could reduce the effects of colloid-facilitated transport—our analysis was conservative.

For the scenarios considered, our results indicate that colloids could be transported through the unsaturated zone and, in this way, influence actinide transport. However, the lack of site-specific data results in a large number of assumptions in the models. Therefore, the most important conclusion from our work is that colloids are an important issue for actinide transport and additional data are needed to properly evaluate the level of risk for colloid transport through the unsaturated zone at Yucca Mountain.

Consequences of Basaltic Magmatism for the Potential Repository

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Yucca Mountain is in a region that has experienced the sporadic formation of small-volume basaltic volcanoes during the past four million years. Because of this, it is necessary to assess the risk posed by magmatic activity at or near the potential repository during its regulatory "lifetime" of 10,000 years. Risk assessment is the product of the probability of a magmatic event intersecting the repository and the consequences of that event. Expert elicitation was used to derive distributions of event probabilities that included varying interpretations of the timing of magmatic events in the region and of the geologic controls on the spatial distribution of volcanoes. These event probabilities were then combined with information on the geometry of volcanic plumbing systems and the layout of the repository to derive the probability that a magmatic event will intersect the potential repository. Based on this work, we estimate that the mean probability of intersection is 1.6×10^{-8}/year. Consequence analysis requires knowledge of the phenomena that will be associated with a possible future eruption. We assume that future eruptions will be similar to the Lathrop Wells volcano (c. 80,000 years old). This forms the basis for probability distributions of major element and volatile compositions (dominated by H_2O, which likely lies between 1 and 3 wt%), as well as magma density and viscosity. We assume that an igneous event that is sufficiently shallow (350 m) to intersect the potential repository will always result in eruption. The event will be characterized by the propagation of a dike set from depth, followed by focusing of flow into one or more roughly cylindrical conduits. Estimated conduit diameters range from 15 to 150 m with a mean of 50 m.

For events where an eruptive center and conduit form at the potential repository, we assume that all waste packages intersected by the conduit are damaged and erupted. Although an actual eruption would have phases of relatively low-violence activity, we simplify the calculations so that all entrained waste is dispersed in an explosive eruption column with characteristics that are determined by observations of analogous eruptions historically around the world. Atmospheric dispersion calculations by collaborators at Sandia National Laboratories predict a mean ash thickness of 2.3 cm and a mean radionuclide concentration of 2.8×10^{-6} g/cm^2 at 20 km from the volcanic vent. For repository designs that include backfill, we predict that disruption will be limited to three waste packages on either side of a dike. For designs where drifts have no backfill, a larger number of waste packages could be damaged. Radiological consequences from subsequent groundwater transport may be as important as those from eruptive dispersal. Our ongoing work is aimed at providing refinements to the geological information used in risk assessment and supporting the Site Recommendation and License Application phases of the YMP.

Volcanism Framework for Probability Calculations

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We completed volcanism research for the YMP in 1996. Our work included site characterization studies and calculations to estimate the probability of disruption of the proposed Yucca Mountain repository. Our results—that the probability of disruption of the repository in the next 10,000 years is 10^{-8} per year—were confirmed by a DOE-sponsored expert elicitation panel, composed of 10 leading independent volcanologists.

In 1999, we were asked to conduct additional research to provide regulatory support for the YMP Site Recommendation Report and the YMP License Application. During this period, we developed and documented an integrated conceptual model of volcanism. We then collaborated in generating revised probability models that account for the recent changes in repository design and recent advances in understanding of the tectonic and volcanic setting of Yucca Mountain.

Field Studies at Yucca Mountain

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Field studies at the potential high-level radioactive waste repository at Yucca Mountain, Nevada, range from surface boreholes drilled into the mountain to elaborate underground test facilities. These studies have characterized the mountain's lithostratigraphy, mineralogy, and hydrologic properties and provided on-site field testing of, for example, the thermal-mechanical properties of the rock and radionuclide transport in the unsaturated zone. This project is discussed in detail in the Research Highlights section.

Managing YMP Facilities and Data

The Engineered Barrier System (EBS) Field Testing Program

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There are several field tests being conducted at Yucca Mountain to test engineered, as opposed to natural, barriers. Formally termed the engineered barrier system, the EBS includes any component installed between the emplacement drift wall and the waste package that would enhance the performance of the overall emplacement system. For example, the EBS could be enhanced by diverting water away from the waste package, disposing of the diverted water from the EBS environment, or maintaining an overall benign environment for the waste package. The EBS field-testing program includes a variety of experiments, from bench-top to quarter-scale. Four field-test activities are presently underway: (1) testing of soil properties in a laboratory environment, (2) a small-scale thermal-hydrological-chemical test, (3) 1.4-m-diameter thermal tests on various drip shield and backfill concepts, and (4) construction of a 40-m-long thermal/ventilation experiment. Unlike most other field tests at Yucca Mountain, the EBS tests are conducted at a DOE facility in North Las Vegas, 90 miles from the Yucca Mountain site. This location and unique test arrangements make for some distinctive test coordination challenges. As is in place for tests near Yucca Mountain, the Test Coordination Office plans and coordinates the EBS work under a fully qualified DOE Quality Assurance Program. The staff prepares field-work packages for the following: (1) facility-design/construction interface, (2) management roles and responsibilities during a test, (3) test requirements, (4) ES&H controls, and (5) budget and schedules.